LA-UR-20-26724
Approved for public release; distribution is unlimited.

Title: Introduction to HE work in XCP-4

Author(s): Meyer, Chad D.

Intended for: Recruitment material for XCP-4

Issued: 2020-08-31

Introduction to HE work in XCP-4

XCP-4: Continuum Models and Numerical Methods

High Explosives sub-team

Chad Meyer

8/17/2020

High Explosives in XCP-4

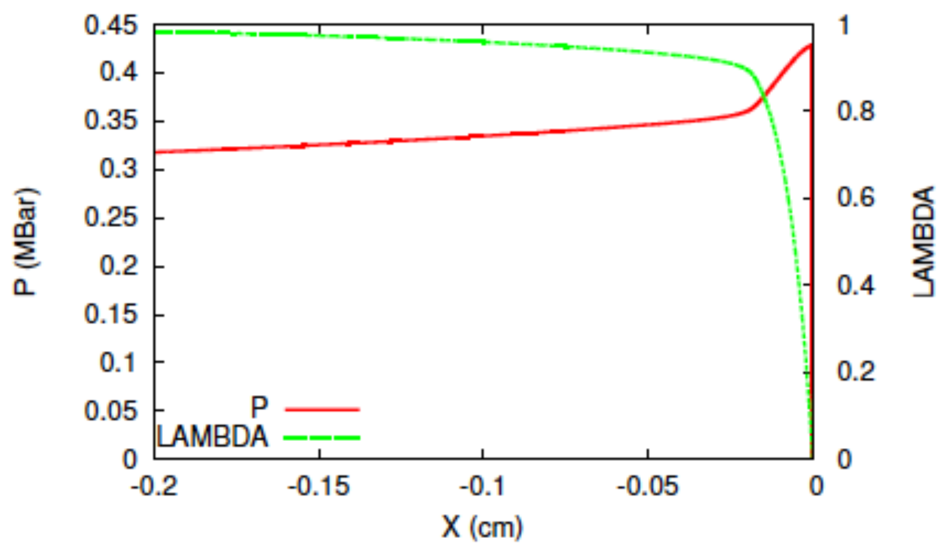
- XCP-4 has a robust and wide-ranging effort to model High Explosives (HEs) in the continuum multiphysics context
  - Model development
  - Implementation of the models in production codes
  - Verification and Validation
  - Modeling of experiments
- We have about 10 people in the sub-group, but most of us are also part of a different sub-group as well
- There are other divisions who also working on explosives science
  - There is also overlap and we work together!
  - M-division does HE experiments, and HE formulation
  - T-division does fundamental science, molecular dynamics, EOS development, model development

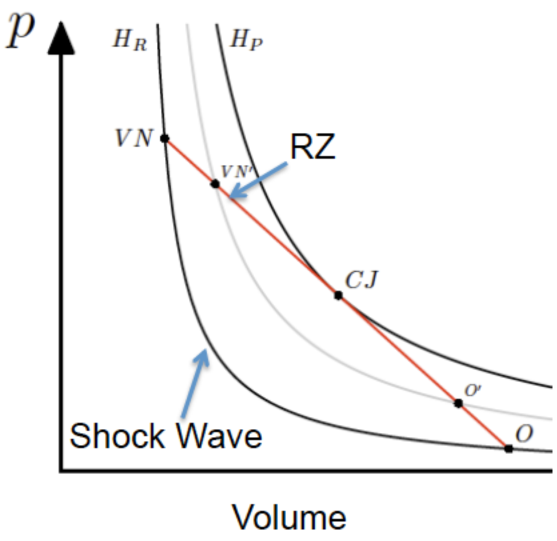
Why model high explosives? Why XCP?

- High explosives are an important part to various parts of the Lab's national security mission
  - Both explosives performance and explosives safety
- Accurate, predictive, HE modeling is challenging!
  - Length scale disparities
    - An average experiment is 10s of cm in size
    - The half-reaction width might be ~50 microns
    - For an insensitive high explosive the reaction might not terminate until ~2000 microns
    - The mean grain size is ~75 microns
  - Sensitivity to initial conditions
    - Initial temperature or density can cause large differences in performance and sensitivity, and even the chemical pathway taken
  - Detonation is very tightly coupled between chemistry and hydrodynamics
- **We want to be able to have a predictive capability**

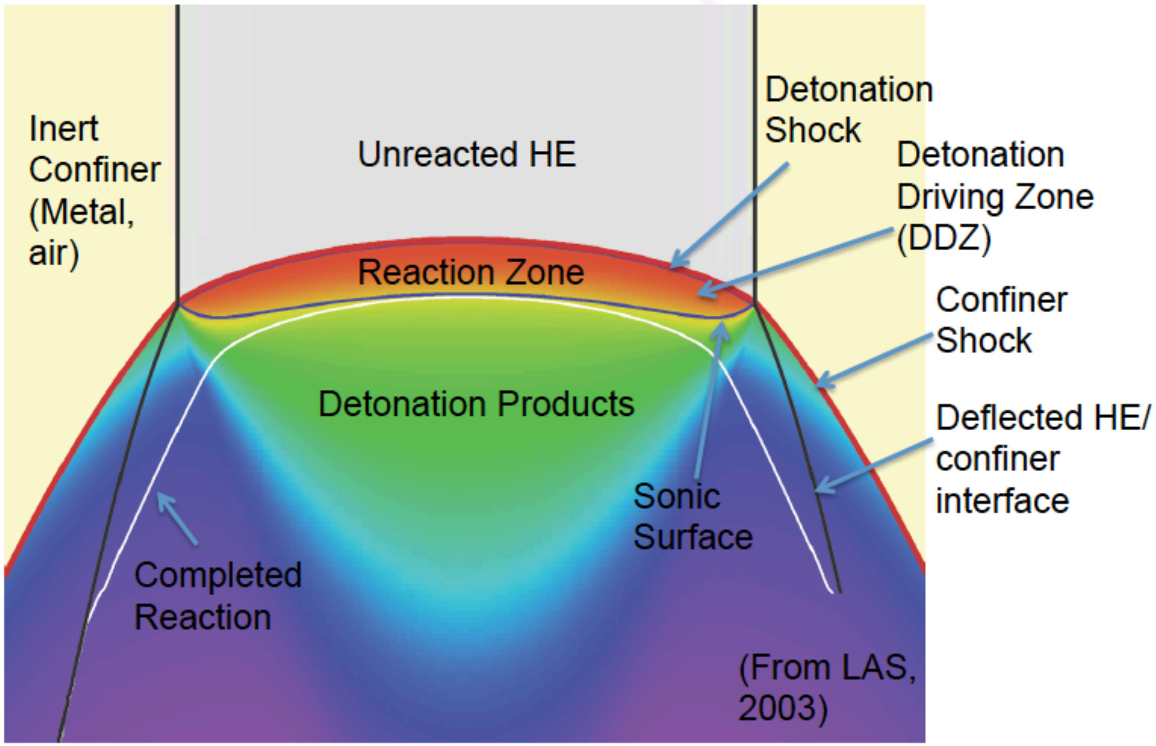
(Extremely Brief) Introduction to HEs

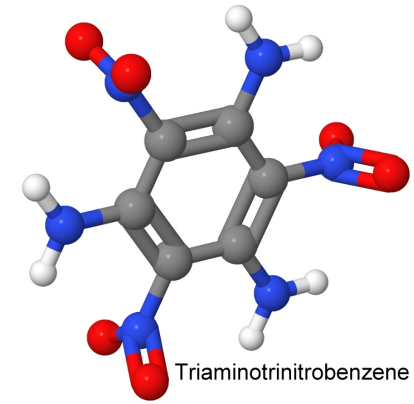
- In 1-D, detonations go at a speed related only to the energy release
- The chemical reaction drives the shock forward
  – It is isolated from the rest of the flow because the shock is supersonic

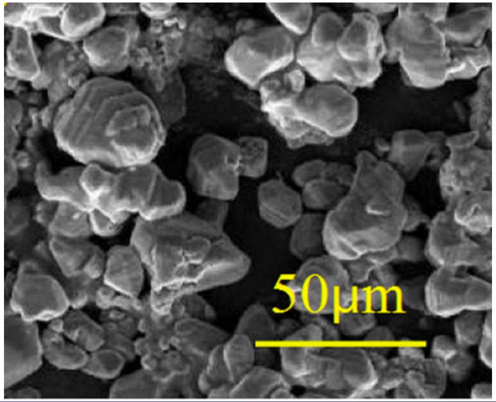




In 2D: some energy pushes the walls sideways, slowing and curving the detonation







What do we do in XCP-4 related to HEs?

- Our biggest responsibility is implementing and maintaining HE models in our production multiphysics codes
  - Burn models
  - Equations of State and multi-material closure
  - Verification and validation of the models
  - Legacy models
- Have to understand the interaction between the HE energy release and other physics packages (across different codes)
  - Strength and damage of metals
  - Hydrodynamics
  - Numerical models
- Expertise to users of the codes, and to model developers

Forward looking HE science

- More advanced continuum burn models
  - Temperature aware
  - More complicated chemistry (most of our models are A→B)
  - Porosity aware
  - [...]
- Microstructure aware modeling; mesoscale level modeling
  - How does this couple to the continuum scale?
  - Why do our continuum scale models do as well as they do?
  - Anisotropic material structure
- New formulations and new lots of old formulations
- Working closely with the materials physics modelers because the details of HE models strongly affect the details of metal deformation

XCP-4: The model integrators

- The group has broad expertise
  - This includes various areas of expertise (hydrodynamics, turbulence, numerical methods, HEs, materials…)
  - It also includes work on and familiarity with multiple code projects
  - This gives us a broader understanding as individuals and as a group
- We have different kinds of hydrodynamics schemes in our production and research codes
  - Lagrangian/ALE/Lagrange+Remap
  - Eulerian/finite volume
  - Discontinuous Galerkin
  - Various other high order approaches
- Integrating the HE models consistently, stably and accurately is one of the *numerical* challenges we face